Theoretical Investigation of the Hydroxylation Mechanism by Cytochromes P450

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Appendix 1. Abbreviations and Acronyms

AMBER	assisted model building with energy refinement; a MM-force field
B3LYP	hybrid density functional consisting of 20% Hartree-Fock and 80% Becke88 exchange combined with the Lee-Yang-Parr correlation functional
BLYP	GGA density functional consisting of the Becke approximation for exchange and the Lee-Yang-Parr functional for correlation
BP or BP86	GGA density functional consisting of the Becke approximation for exchange and the Perdew expression for correlation
cam	camphor
CASPT2	Complete Active Space with Second-order Perturbation Theory
CASSCF	Complete Active Space Self-Consistent Field Theory
cc-pV(D,T,Q)Z	correlation-consistent polarized (double, triple, or quadruple)-split valence basis set
CHARMM	chemistry at Harvard molecular mechanics; a MM-force field
CI	configuration interaction (a post Hartree-Fock method)[376]
DFT	density functional theory
DZ	double zeta (basis set)
DZP	double zeta + polarization (basis set)
ENDOR	electron-nuclear double resonance spectroscopy
ESR	electron spin resonance spectroscopy
G2	Gaussian-2 theory (the second in a series of Gx methods for calculation of total energies of a given molecular species using a composite technique in which a sequence of well-defined ab initio molecular orbital calculations is performed)[199]
G3	Gaussian-3 theory (the third in a series of Gx methods for calculation of molecular energies, see also G2)[200]
GGA	generalized density gradient approximations
HF	Hartree-Fock

HOMO	Highest occupied molecular orbital
KIE	kinetic isotope effect
kx	rate constant for a certain reaction x
LACVP	Los Alamos Effective Core Valence Potential (basis set)
LDA	Local density approximation
LUMO	Lowest occupied molecular orbital
LYP	Lee-Yang-Parr Correlation functional
meta-GGA	Meta Generalized Gradient Approximation
MM	molecular mechanics
MO	molecular orbital
MRMP	multireference Møller-Plesset
OPLS	optimized potentials for liquid simulations
OPTX	Handy-Cohen Optimized Exchange Functional
P450	Cytochrome P450 protein
PBE	Perdew–Burke–Ernzerhof Correlation functional
SCF	Self-Consistent Field approach; in an SCF calculation the wavefunction is gradually refined until self-consistency is achieved
STO	Slater type orbital
THF	tetrahydrofuran (oxacyclopentane)
TZ	triple zeta (basis set)
TZP	triple zeta + polarization (basis set)
ZORA	a relativistic zeroth-order regular approximation